DEVELOPING A FRAMEWORK FOR PERFORMING HIGH-FIDELITY ENGINE SIMULATIONS USING NEK5000 CODE FOR EXASCALE COMPUTING

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Project ID # ACE126

OVERVIEW

Timeline

- New project funded in FY19
- Project start date: July 2018

This project is now part of the "Advanced Light-Duty Combustion Consortium" (FY19-24)

Barriers

Lack of robust combustion technology for advanced dilute combustion SI engines:

- Incomplete understanding of the dynamics of fuel-air mixture preparation
- Incomplete understanding of stochastic combustion problems (CCV, misfire, knock)
- <u>Lack of a truly predictive simulation tool for engine design</u>

Budget

- FY 18: $400 K
- FY 19: $700 K

Main Partners

Current partners:

- Paul Fischer (UIUC)
- Joe Insley, Silvio Rizzi (ANL-LCF)

In discussions with several laboratory and university PIs to establish partnership

BACKGROUND AND OBJECTIVES

- Current status of engine simulation codes:
  - Low-order numerical schemes – large numerical dissipation
  - Poor scalability – cannot effectively utilize future exascale systems
  - Simplified turbulence, spray and combustion models
- Existing codes need significant model tuning to match experimental data – not truly predictive
- Nek5000 is an open-source, massively parallel, high-order CFD code that already has capabilities to model in-cylinder engine flows

<u>Objectives:</u>

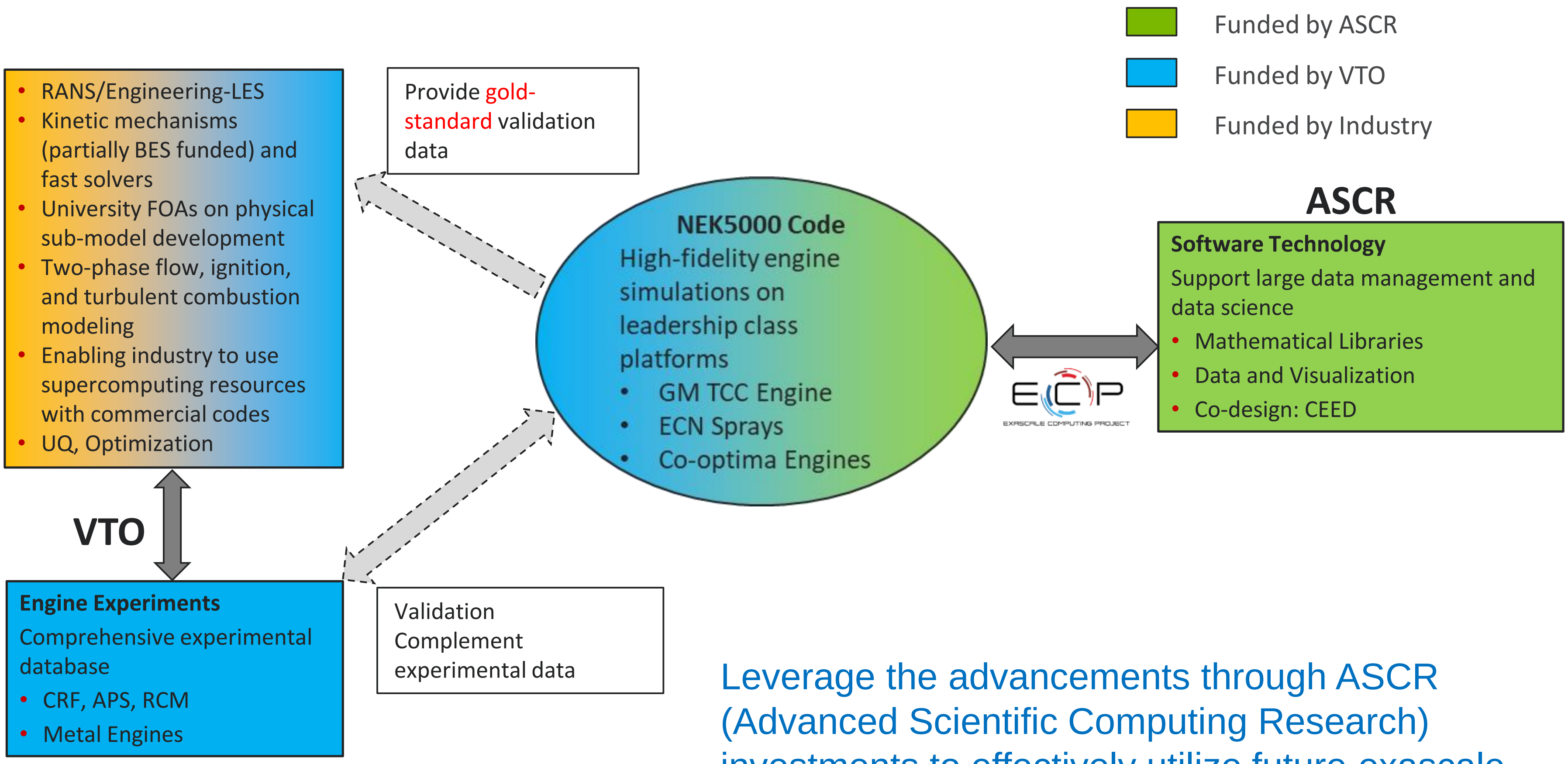
- Adapt Nek5000 code into a simulation platform tailored for ICE simulations:
  - Conduct DNS and high-fidelity LES simulations– provide detailed numerical data that can complement experiments
  - Provide an accurate platform for testing and developing ICE-specific turbulence, spray and combustion submodels
- Identify the root causes of cyclic variability and provide the understanding needed to design for their minimization

RELEVANCE

- DOE VTO workshop (2014) identified "Accuracy, speed, and availability" as key requirements for future CFD activities
- Nek5000 code development supports these objectives:
  - Accuracy: High-order features of the code leads to very accurate prediction of in-cylinder flow features
  - Speed: ASCR investments through ECP used to ensure high scalability on current and future computing architecture
  - Availability: Open-source and easily available for industry and academia
- Advanced Light-Duty Combustion Consortium identified "Cyclic variability mitigation" as one of the key purposes
- Modeling tools can be used to identify sources of CCV and develop and evaluate potential mitigations
- To accurately predict CCV, the CFD tool needs to accurately predict cycle-to-cycle variations in in-cylinder flow and mixing processes – needs high fidelity simulations
- Nek5000 simulations will provide detailed numerical data that are impossible to obtain with experiments alone
  - Support engineering sub-model development
  - Allow the latest ML tools to discover hidden relationships

RELEVANCE

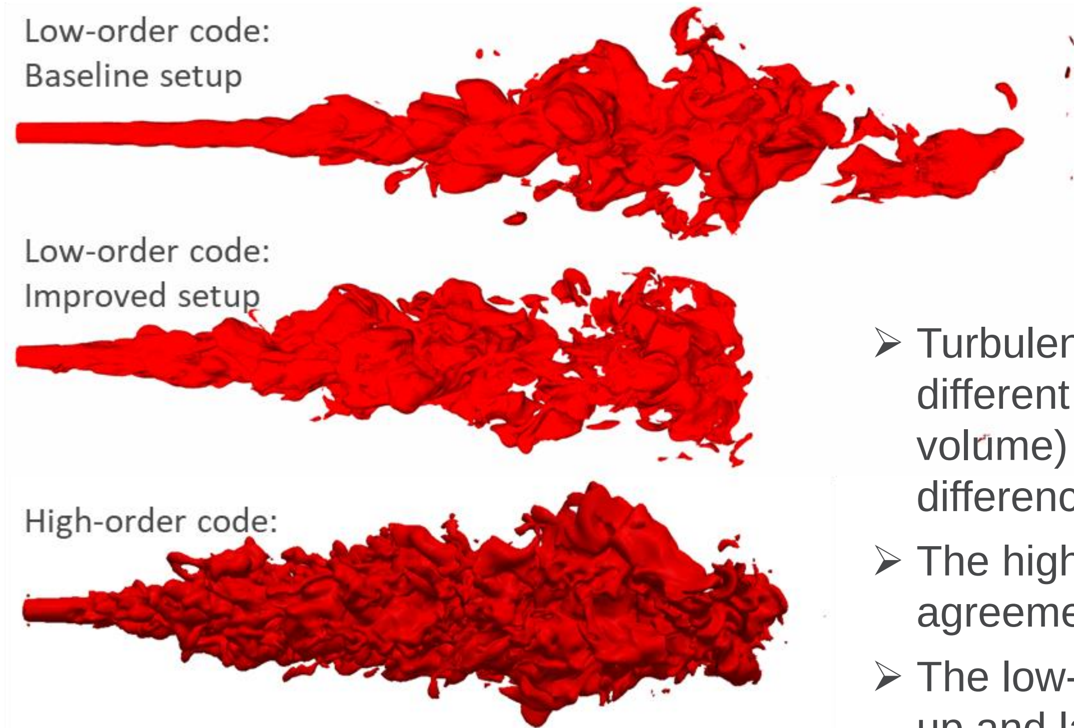
A NEW PARADIGM OF COLLABORATION BETWEEN VTO AND ASCR



Leverage the advancements through ASCR (Advanced Scientific Computing Research) investments to effectively utilize future exascale resources to perform high-fidelity ICE simulations

RELEVANCE – WHY HIGH ORDER?

HIGH-ORDER CODES IMPROVE LOW-ORDER CODES



Case	Potential Core Length (d_j)	Spreading Rate (S)
Experiment	6.2	0.094-0.102
High-order	5.5	0.104
Low-order	15.5	0.115
Low-order (improved)	6.6	0.0997

Wang, Ameen et al* showed how high-order simulation results can be used to improve the performance of low-order codes

- Turbulent round jet was modeled using two different codes - a low-order (2nd order finite volume) and a high-order (6th order finite difference) code
- The high-order code showed excellent agreement with the experiments
- The low-order code showed earlier jet break-up and larger spreading rates
- High-order code simulations motivated improvements in the low-order code setup (inflow perturbations and subgrid model)
- The improved low-order code showed similar jet structure as the high-order code

*Wang, Z., Ameen, M., Som, S., and Abraham, J., *SAE Int. J. Commer. Veh.* 10(2):2017, doi:10.4271/2017-01-0575.

MILESTONES

FY19

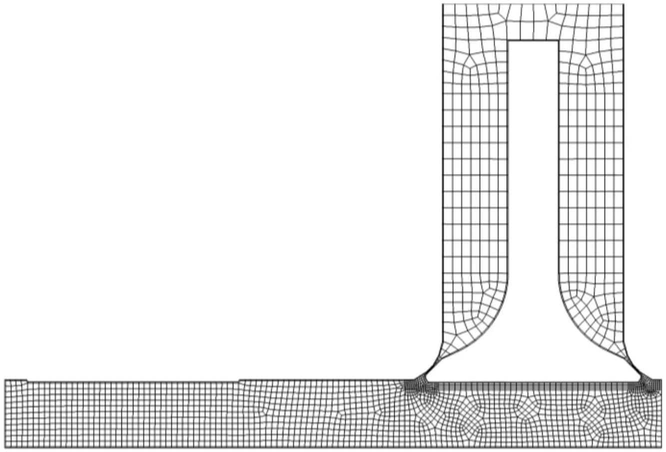
- Q2 FY19: Perform LES of turbulent non-reacting jet and validate against experimental measurements [completed]
- Q4 FY19: Perform multi-cycle LES of motored TCC-III engine at 500 and 800 rpm [On-track]
  - Overset meshing technique – validation for 2D engine simulations [completed]
  - Perform 3D simulations with spark plug geometry [On-track]
- Q4 FY19: Perform LES of the Cabra flame and validation against experimental measurements [On-track]
  - Develop Low-Mach formulation for flamelet models [completed]
  - Implement PSR and FPV models into Nek5000 [completed]
  - Perform LES of Cabra flame using Nek5000 [On-track]

FY20

- Q2 FY20: Complete implementing spray models and validate with benchmark experiments
- Q3 FY20: Complete implementing ignition, and flame propagation models and validate with benchmark flame experiments
- Q4 FY20: Perform multi-cycle LES of the Sandia optical DISI engine under motored operating condition

SIMULATION APPROACH – NEK5000

- Spatial discretization: Spectral element method (SEM) (Patera 84, Maday & Pater, 89)
  - Solution represented as Nth order tensor-product polynomials inside each element (N~ 5-15)
  - Delivers minimal numerical dispersion and dissipation
  - Exponential convergence with N
- Temporal Discretizations
  - Semi-implicit and characteristic-based schemes (up to 3rd order accurate)
- Body-fitting capabilities for complex geometries
- Arbitrary Lagrangian Eulerian (ALE) capabilities to handle moving geometries
- Mesh generation: utilities available to convert meshes generated from several 3rd party mesh generators (ICEM, CUBIT etc.) to Nek meshes
- High-order grid-to-grid interpolation utility to use several sequential SEM meshes for a transient moving geometry simulation



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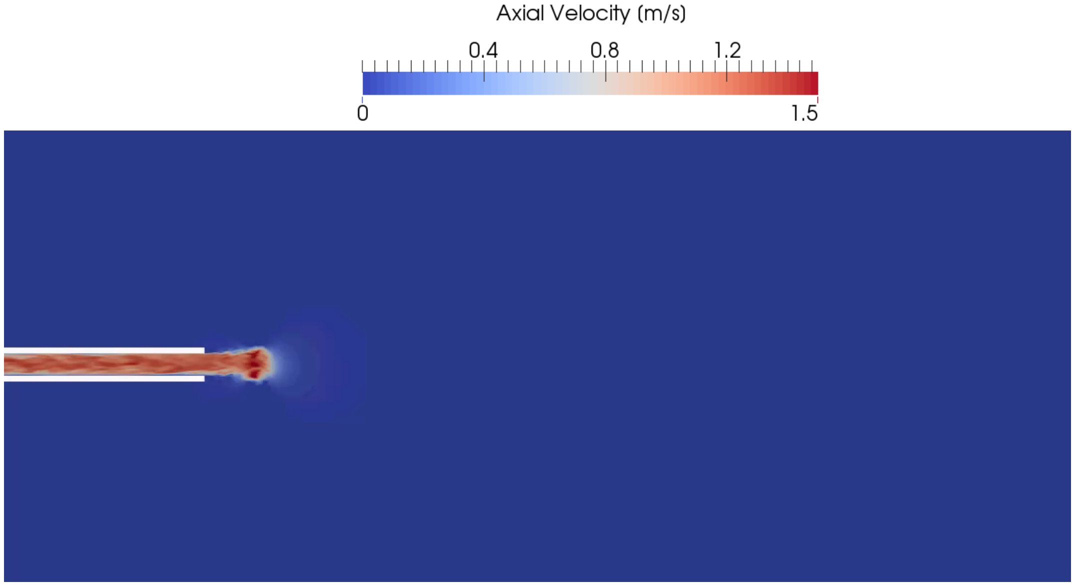
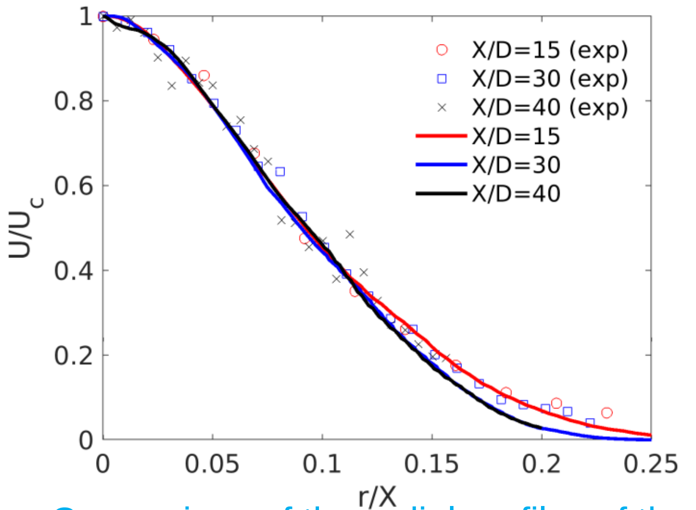
TECHNICAL ACCOMPLISHMENT

TURBULENT JET FLOW SIMULATIONS



Video showing the non-dimensional axial velocity in the near-field of the round jet (Re=5500)



Comparison of the radial profiles of the mean axial velocities at different axial locations from the simulations and experiments (Vouros and Panidis (2004))

Case	Polynomial order (N)	No. of Filtered Modes	Spreading Rate
Exp			0.08
Sim 1	5	2	0.1222
Sim 2	7	2	0.0846
Sim 3	7	3	0.0964

- Parametric study of polynomial order, grid size, and filtering scheme was performed
- Polynomial order showed the strongest effect on jet structure
- Performance of low-order codes can be improved based on these results
- Simulation results will be presented at the ASME ICEF 2019

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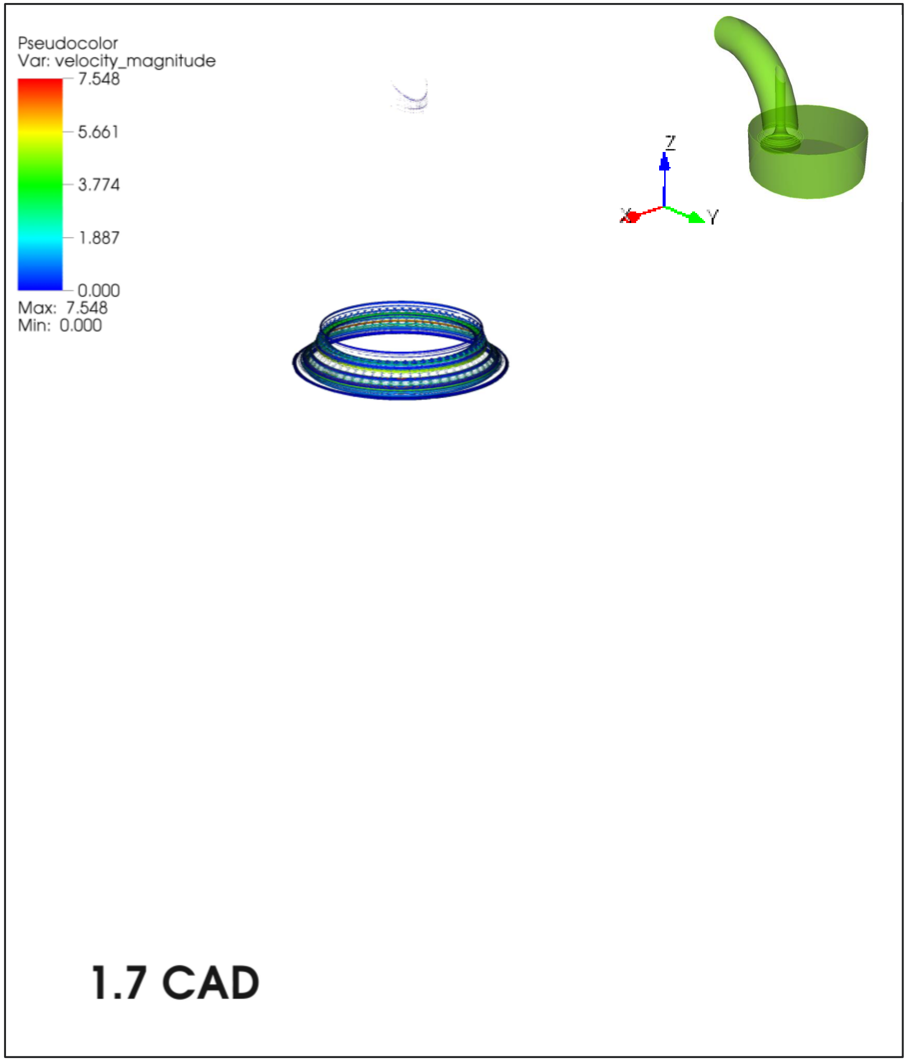
TECHNICAL ACCOMPLISHMENT

INTAKE STROKE OF 3D TCC-III MOTORED OPERATION @ 500 RPM (1/2)

Resolution Parameters	
Polynomial Order (N)	7
Min # of Elements	79 K Elements at ~TDC
Max # of Elements	163 K Elements at BDC
Min # of Total Points @ TDC	**27.5 M**
Max # of Totals Points @ BDC	**56.5 M**
Element Size (h)	0.2 - 1.1 mm (TDC → BDC)
Effective Resolution O (h/N²) – O (h/N)	0.004 – 0.15 mm

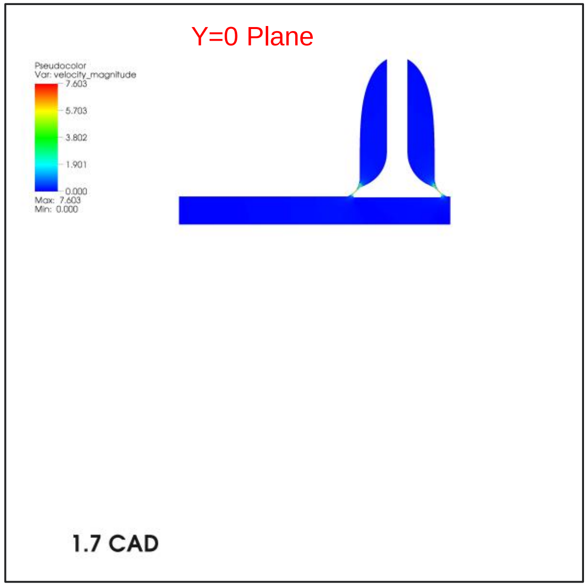
- 6 SEM grids constructed a-priori in CUBIT
- High-Order grid-to-grid interpolation was utilized to progress the simulation
- Characteristic (semi-Lagrangian) time-stepping for ALE (**Patel et. al 2018**)
  - CFL = 3.0
- Projected Performance of ~7 Wall-Hours on 256 Nodes (16K processors) of Theta supercomputer at ANL

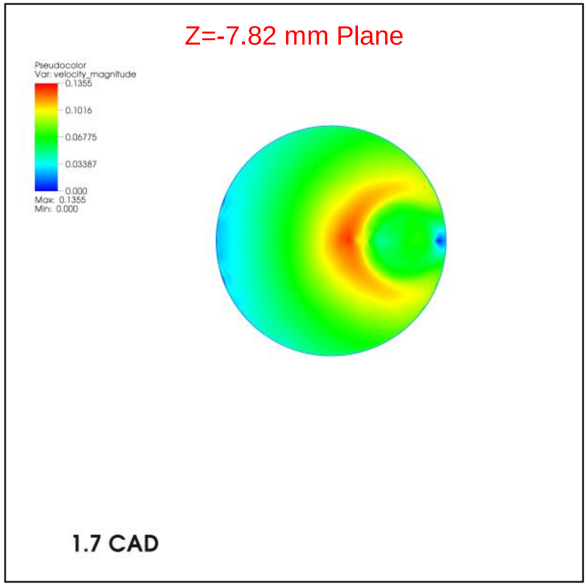


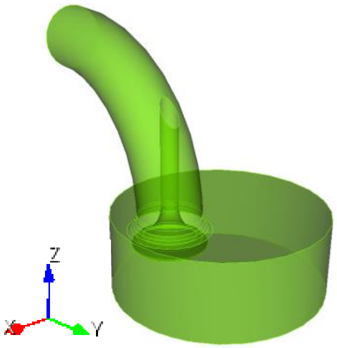
TCC-III (no-spark): λ_2 vortices (Jeong & Hussein '95) appearing during the intake stroke.

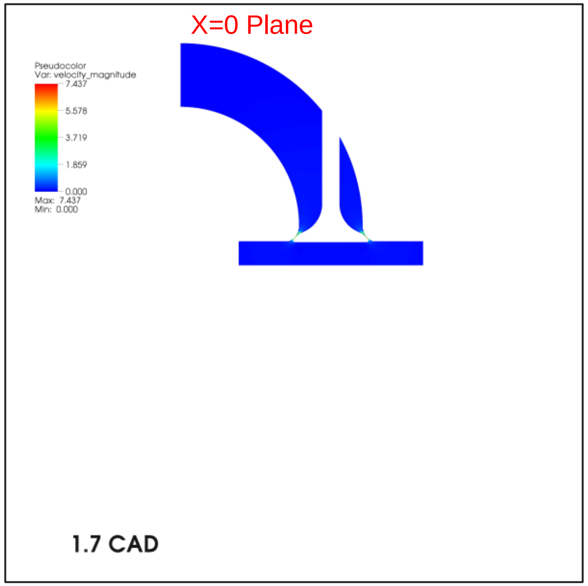
TECHNICAL ACCOMPLISHMENT

INTAKE STROKE OF 3D TCC-III MOTORED OPERATION @ 500 RPM (2/2)





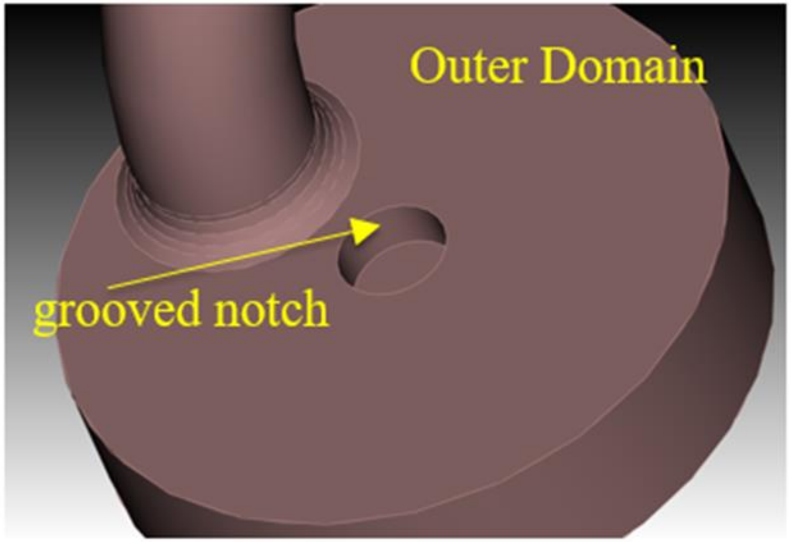


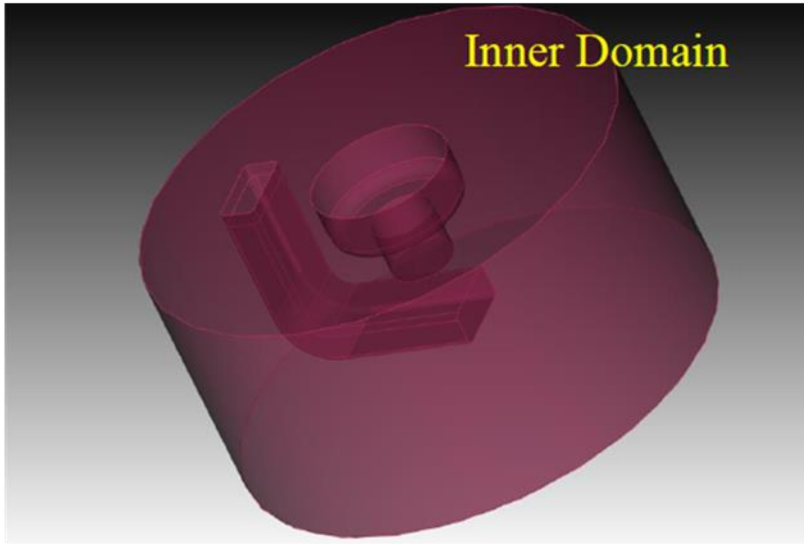


- Demonstrated simulation workflow to perform 3D engine simulations using Nek5000
- Preliminary simulations without the spark plug geometry were performed
- Simulations show the turbulent intake jet structure and the in-cylinder flowfield
- Including the spark plug geometry in the simulations is challenging and this requires the use of overset meshing strategy

TECHNICAL ACCOMPLISHMENT
OVERSET MESHING STRATEGY

- Current meshing challenges using Nek5000:
  - Meshing the spark plug region is very challenging
  - As the valve moves, the mesh near the spark plug can become distorted
- Strategy:
  - Use NekNek overset meshing strategy
  - Two separate spectral element simulations running concurrently and exchanging data at the interfaces of the overlap region
  - Fixed mesh around the spark plug and a moving ALE mesh in the rest of the geometry





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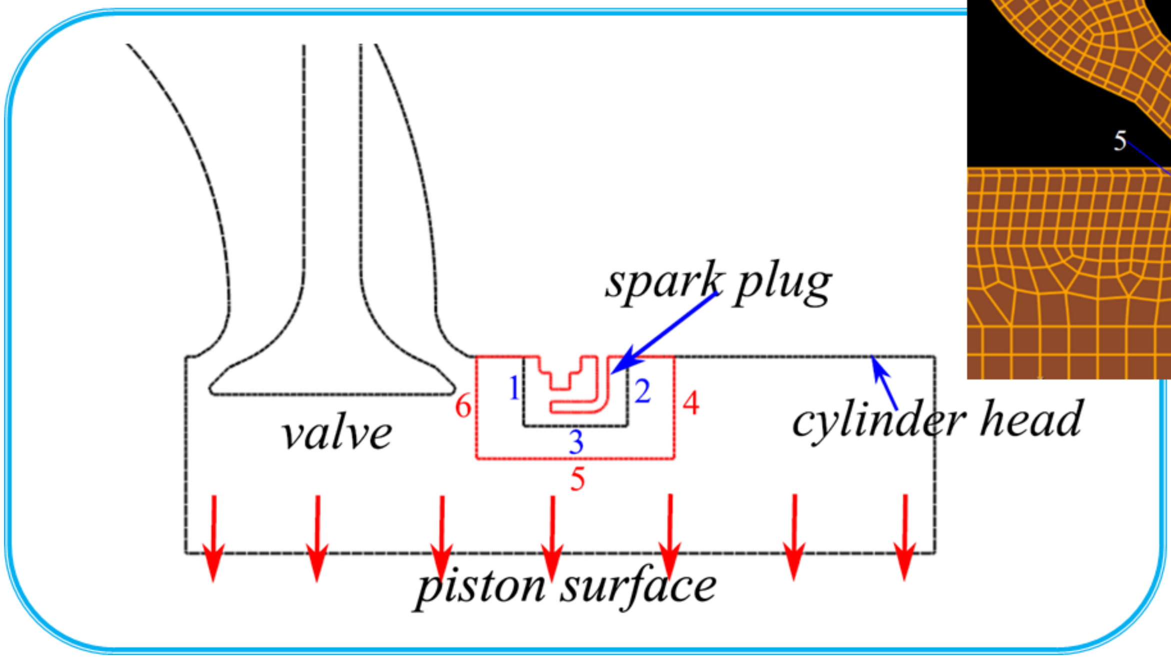
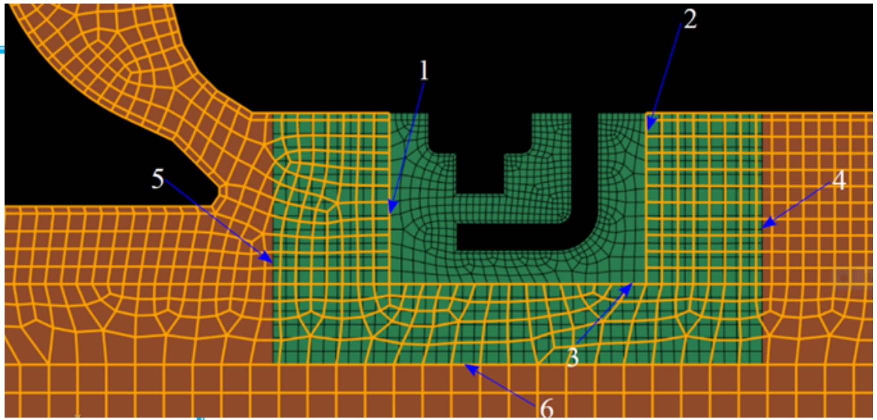
TECHNICAL ACCOMPLISHMENT

VALIDATION OF OVERSET MESHING STRATEGY FOR TCC-III (1/2)

- The domain is created from a 2D projection of the 3D TCC-III engine model on an xy plane corresponding to the crank angle in degrees (CAD) of 45.
- Only consider piston motion; valve is completely open
- One standard single mesh case and two different NekNek cases with large and small areas of overlap (Meshes carefully designed to have very similar mesh topology, mesh sizes, and mesh counts for all 3 cases)

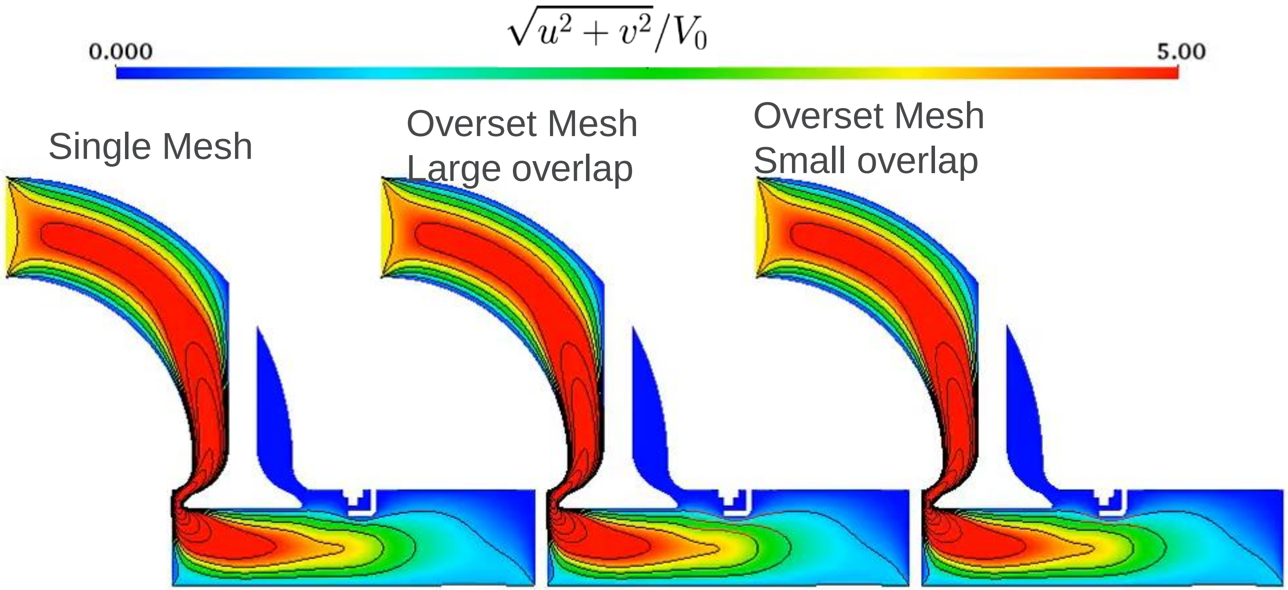
Schematic of Overlapping grids

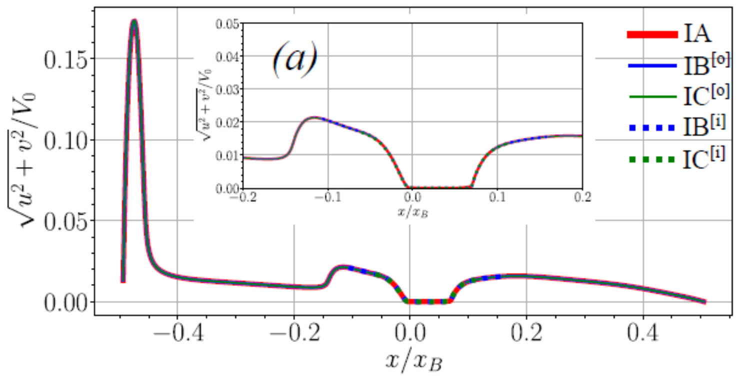




TECHNICAL ACCOMPLISHMENT

VALIDATION OF OVERSET MESHING STRATEGY FOR TCC-III (2/2)





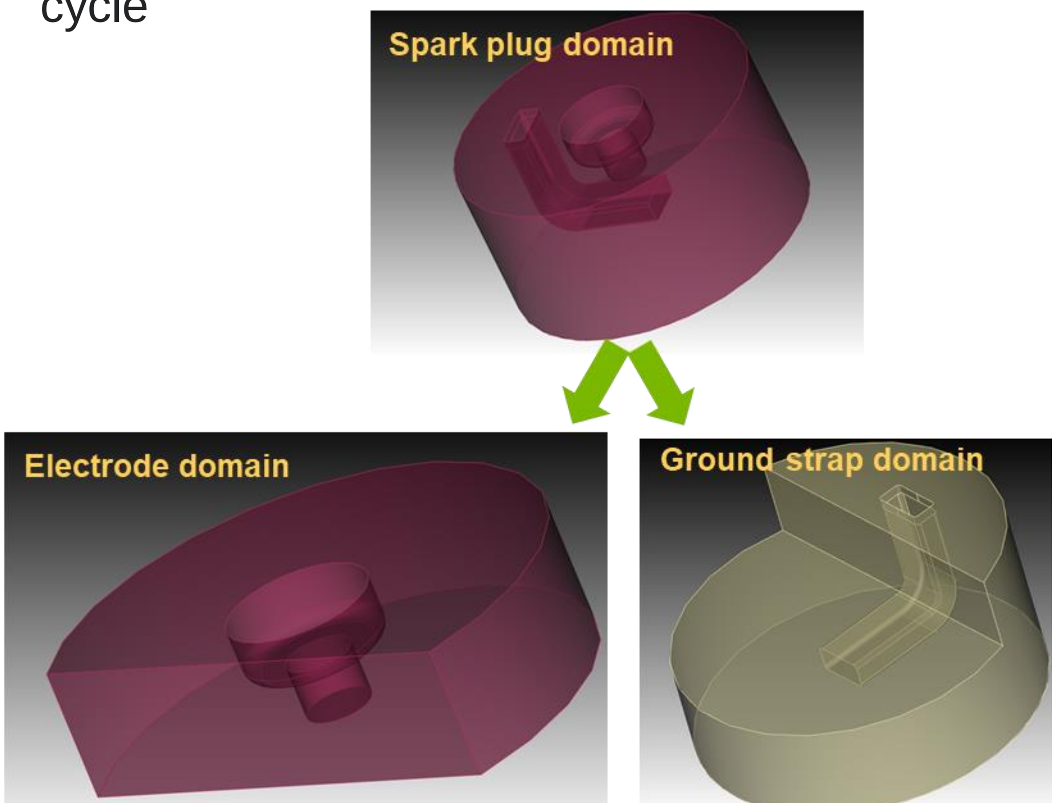
- Overall good agreement between the single mesh and overlapping mesh simulations
- Demonstrated the feasibility of overset meshing for ICE simulations
- Next Step: Perform 3D simulations of TCC-III using the overset meshing strategy

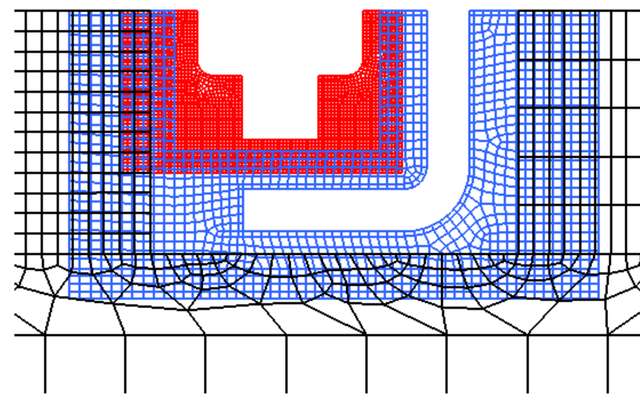
*T Chatterjee, SS Patel, MM Ameen (2019) “Towards improved mesh-designing techniques of spark-ignition engines in the framework of spectral element methods” presented at the US National Combustion Meeting, March 2019

TECHNICAL ACCOMPLISHMENT

EXTENDING THE OVERSET MESHING STRATEGY

- NekNek approach was further extended to performing more than 2 concurrent simulations.
- Currently exploring a strategy with 3 overset domains (NekNekNek) where the inner domain containing the spark plug is further broken down into two overlapping subdomains
- This strategy leads to an improved control on mesh sizes throughout the engine cycle





Interfaces/overlap between the outer domain (black), ground strap domain (blue), and electrode domain (red)

TECHNICAL ACCOMPLISHMENT

COMBUSTION MODEL IMPLEMENTATION (1/3)

- Two different combustion models have been implemented – a perfectly stirred reactor (PSR) combustion model and a tabulated flamelet progress variable (FPV) model.
- PSR model involves solving transport equation for each chemical species
- Chemical source terms evaluated using a Chemkin library which is completely linked with Nek
- Thermal divergence term (relevant for low Mach applications) evaluated using:

$$Q_T = \frac{1}{\rho}\sum_{i=1}^{N_g}\frac{W}{W_i}\left(-\nabla\cdot\rho D\nabla Y_i + \dot{\omega}_i\right) + \frac{1}{\rho c_p T}\left(\nabla\cdot(\lambda\nabla T) - \sum_{i=1}^{N_g} h_i\dot{\omega}_i\right)$$

- For FPV model implementation, species transport equations are not solved; a new formulation for Q_T was derived (c, Z are progress variable and mixture fraction) and implemented into Nek5000

$$Q_T = F_1(c,Z) - F_2(c,Z)|\nabla c|^2 - F_3(c,Z)(\nabla c)\cdot(\nabla Z) - F_4(c,Z)|\nabla Z|^2 + \frac{1}{T}\omega_T + \frac{1}{\rho c_p T}\nabla\cdot(\lambda\nabla T)$$

Where

$$F_1(c,Z) = \sum_{i=1}^{N_g}\frac{W}{W_i}\dot{\omega}_i$$

$$F_2(c,Z) = \sum_{i=1}^{N_g}\frac{W}{W_i}\frac{\partial}{\partial c}\left[\rho D\frac{\partial Y_i}{\partial c}\right]$$

$$F_3(c,Z) = \sum_{i=1}^{N_g}\frac{W}{W_i}\left\{\frac{\partial}{\partial Z}\left[\rho D\frac{\partial Y_i}{\partial c}\right] + \frac{\partial}{\partial c}\left[\rho D\frac{\partial Y_i}{\partial Z}\right]\right\}$$

$$F_4(c,Z) = \sum_{i=1}^{N_g}\frac{W}{W_i}\frac{\partial}{\partial Z}\left[\rho D\frac{\partial Y_i}{\partial Z}\right]$$

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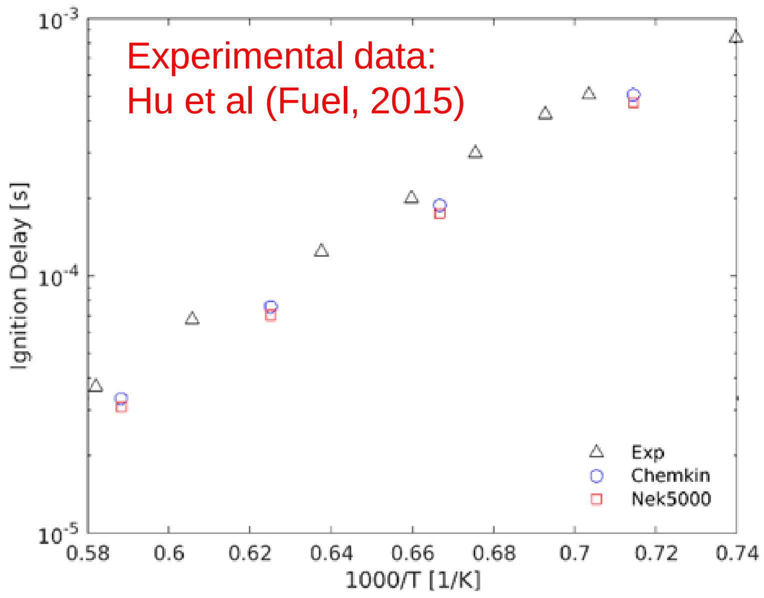
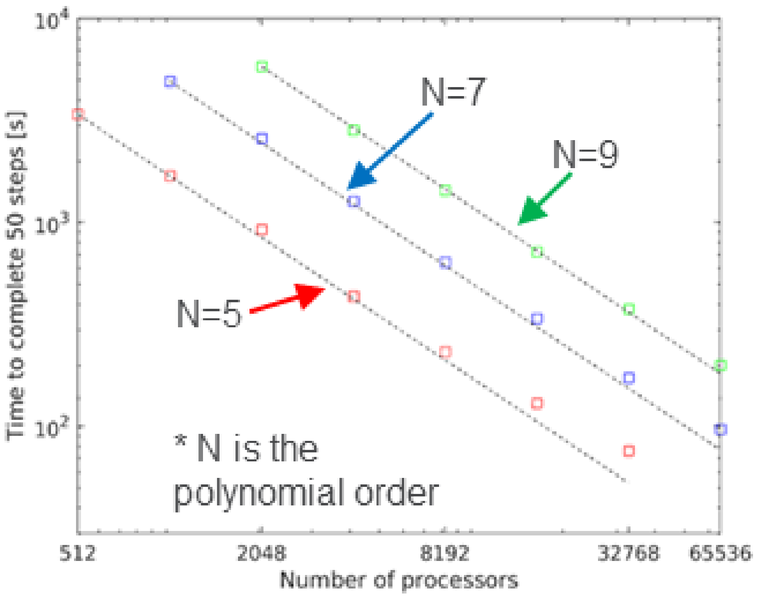
TECHNICAL ACCOMPLISHMENT

COMBUSTION MODEL IMPLEMENTATION (2/3)

- Implementation of PSR model was validated by computing ignition delay of methane/air mixture in a shock tube
- Predicted ignition delays using Nek5000 were comparable to 0D ignition delay predicted by Chemkin
- Excellent strong scaling demonstrated on up to 65,376 processors on ALCF Theta (1/4th of the whole machine)



Ignition delay of methane/air mixtures predicted by Nek5000 with GRI 3.0 mechanism



Strong scaling performance of Nek5000 to simulate 3D reacting mixing layer on ALCF Theta

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RESPONSE TO PREVIOUS YEAR REVIEWERS' COMMENTS

- This project was newly funded in FY19 and was not reviewed last year

PARTNERSHIPS/COLLABORATIONS

Current Collaborators:

- Paul Fischer (UIUC) – Solver development for compressible version of Nek5000
- Joe Insley, Silvio Rizzi (ANL-LCF) – Integrate in-situ visualization capabilities

Potential Collaborators in FY20:

- Riccardo Scarcelli (ANL) – Implement advanced ignition models
- Russell Whiteside (LLNL) – Implement fast chemistry solvers
- Magnus Sjoberg (SNL) – Experimental data from Sandia DISI optical engine
- Sibendu Som (ANL) – Explore hybrid DNS/LES workflow
- Dave Carrington, Jiajia Waters (LANL) – Mesh generation
- Yulia Peet (ASU) – Heat transfer model
- Noah VanDam (UML) – DI spray, UQ
- Convergent Science – Implement improved submodels

- Presentations at Advanced Engine Combustion (AEC) Working group
- Engine Combustion Network Participation and Data Contribution

REMAINING CHALLENGES AND BARRIERS

Model implementation challenges

- Mesh Generation:
  - The overset meshing strategy that is currently employed in Nek5000 for ICE simulations need to be optimized and tested for scalability
- Spray Models:
  - A Lagrangian phase model is already available in Nek5000, however spray specific submodels (collision, breakup etc) need to be implemented and tested
- Ignition and flame propagation models need to be implemented and tested

Practical challenges

- Coupling with commercial CFD codes:
  - Need to develop workflows to perform hybrid DNS/LES or LES/RANS simulations by coupling with commercial or open-source low-order CFD codes
  - Use data generated from Nek5000 simulations to improve submodels in low-order codes
- Proper archival of data:
  - High fidelity simulations will generate several TBs of data. There is a need to develop workflows to properly archive this data for future ML tasks

PROPOSED FUTURE WORK

Remaining Milestones for FY19:

- Q4 FY19: Multi-cycle LES of motored TCC-III engine at 500 and 800 rpm [on-track]
- Q4 FY19: LES of the Cabra flame and validation against experimental measurements [on-track]

Proposed Future Tasks :

- Obtain computing core hours on Theta/Summit using ALCC/INCITE proposals
- Complete implementing spray, ignition, and flame propagation models and validate with benchmark experiments [FY20]
- Perform scalability study for the engine simulations on Theta and identify and solve potential bottlenecks
- Multi-cycle LES of the Sandia optical DISI engine [FY20-FY21]:
  - Improve understanding on causes of cyclic variability in flow, mixing, spray and combustion
  - Archive numerical setup, flow and thermal data
- Develop an easy-to-use, open-source platform that industry/academia/national lab PIs can use for submodel development

Any proposed future work is subject to change based on funding levels

SUMMARY

Relevance:

- Need for predictive, open-source simulation tools to improve understanding of stochastic combustion problems
- High-order CFD codes can provide higher accuracy at lower cost

Approach:

- Use Nek5000, a high-order open-source spectral element code to generate detailed numerical data that are impossible to obtain from experiments alone
- Develop Nek5000 into an accurate platform for testing and developing ICE-specific turbulence, spray and combustion submodels

Accomplishments:

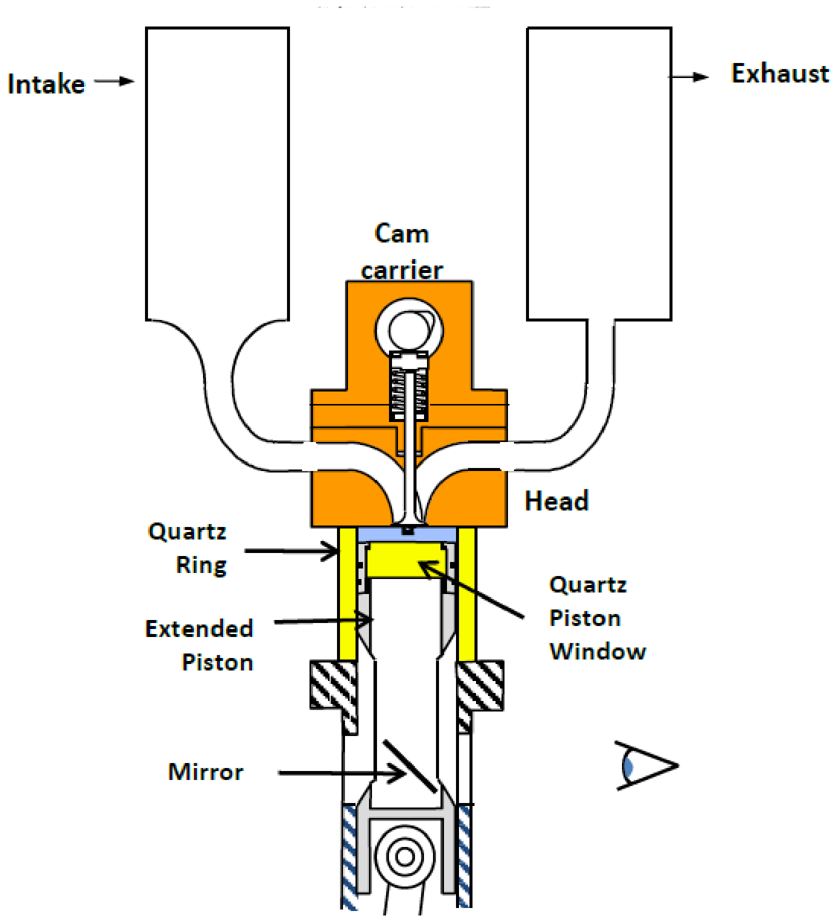
- Performed LES of turbulent non-reacting jet and validated against experimental measurements
- Demonstrated overset meshing technique and validated for 2D engine simulations
- Demonstrated simulation workflow to perform 3D engine simulations
- Implemented PSR and FPV combustion models to Nek5000

Future Work:

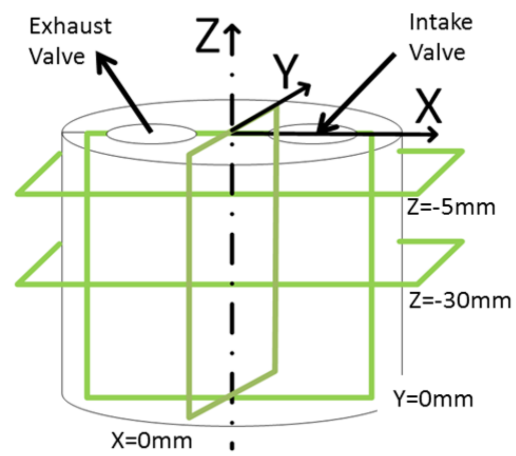
- Multi-cycle LES of the Sandia optical DISI engine and validation with PIV
- Complete implementing spray, ignition, and flame propagation models and validate with benchmark experiments
- Develop an easy-to-use, open-source platform that industry/academia/national lab PIs can use for submodel development

TECHNICAL BACK-UP SLIDES

TCC-III ENGINE EXPERIMENTAL SETUP



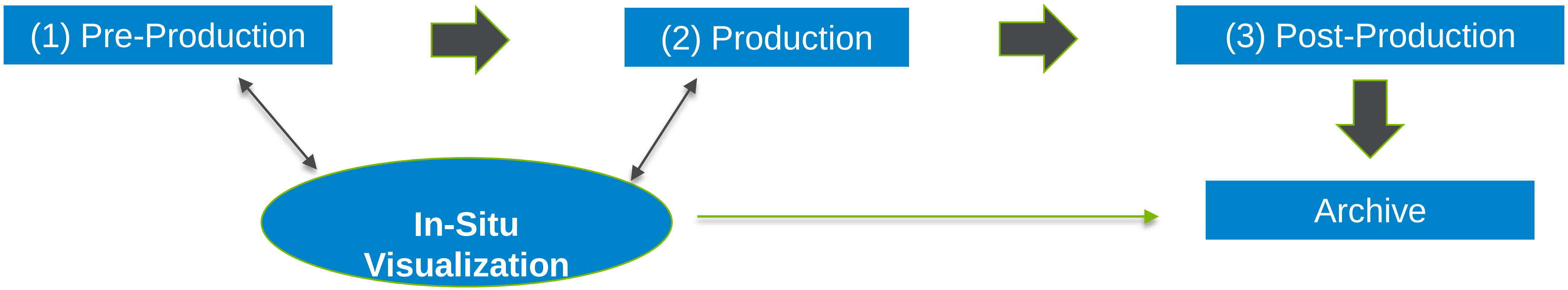
Bore	92 mm
Stroke	86 mm
Connecting rod length	231 mm
Compression ratio	10:1
Intake valve opening	712 deg ATDCE
Intake valve closing	240 deg ATDCE
Exhaust valve opening	484 deg ATDCE
Exhaust valve closing	12 deg ATDCE



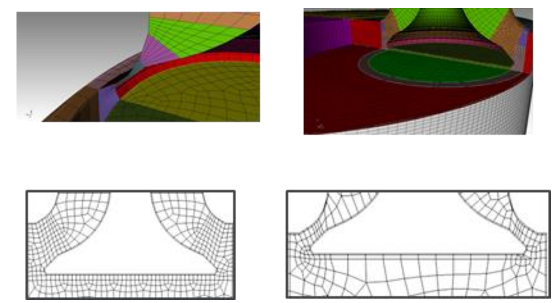
PIV Measurement Planes

*Sick, V. et al., 2010, "A Common Engine Platform for Engine LES Development and Validation," LES for Internal Combustion Engine Flows, Rueil-Maimaison, France.

NEK5000 WORKFLOW FOR ENGINE SIMULATIONS



1. Pre-Production – Mesh generation & stiff solver support



- Using the CUBIT (Sandia) toolkit, we generate multiple body-fitted, HEX27-based meshes which conform to engine boundaries (i.e. piston and valve positions) at every Nth CAD. Each grid will have boundary-layer (BL) resolution using a combination of "pillowing" techniques from CUBIT and skinning subroutines part of Nek5000's toolkit.
- Perform a combination of CUBIT-based and Nek5000-based smoothing techniques to create relatively homogeneous element sizes in the far-field (away from boundaries). This will help to reduce computational cost of stiff pressure Poisson solve.
- Utilize **in-situ visualization** to validate each mesh. Visualize the field of pointwise Jacobians and see where, if at all, they are vanishing thus leading to "mangled" elements.

2. Production – Execute Simulation

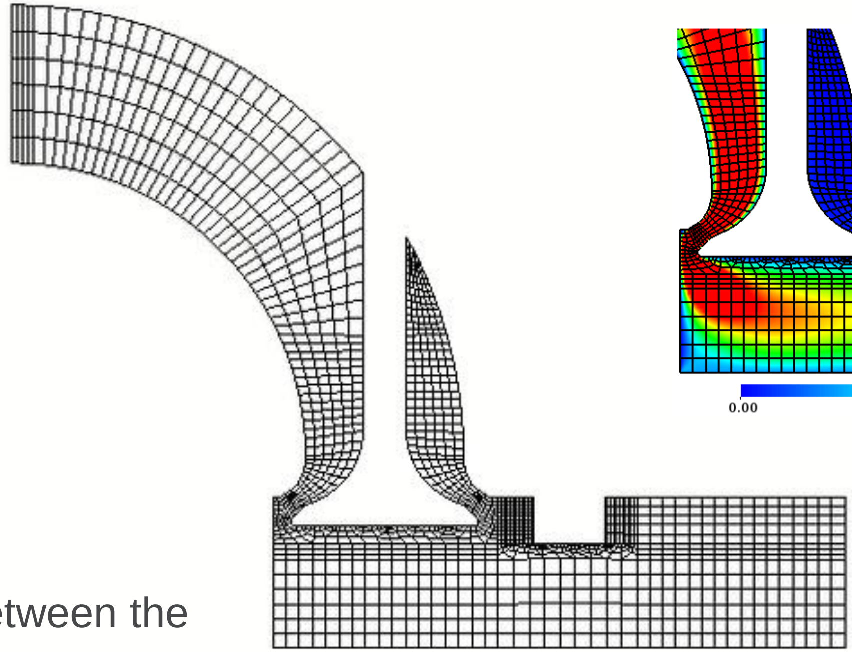
- Submit relevant data files to production queues on ALCF's machine, Theta. Four primary files (`.usr, .re2, .ma2,` and `.par)` contain mesh, boundary, and domain decomposition information. Supporting data files related to relevant species properties can be easily integrated into the workflow.
- Depending upon the problem size (number of elements and RPMs), large-eddy simulations will run on at least 256 nodes of Theta (16K processors). Perform **check-pointing (CP)** to occur at every CAD or ½ CAD. Enable grid-to-grid interpolation to ensure adequate resolution during engine cycle.
- Utilize **in-situ visualization** to render relevant thermal, species, and flow-field characteristics. This would also allow researchers to interactively change view angles, adjust sampling steps, edit color and opacity, and zoom in and out to visually monitor simulation runs. Some suggestions for the TCC-III would include visualizing 2D "slices" of the velocity magnitude at every timestep thereby allowing investigation of the flow at an inter-CP frequency. Additional possibilities include volume rendering of selected species undergoing combustion. Images can be immediately archived to storage for later use. Two main software applications are **VisIT** and **ParaView**.

3. Post-Production – Analysis

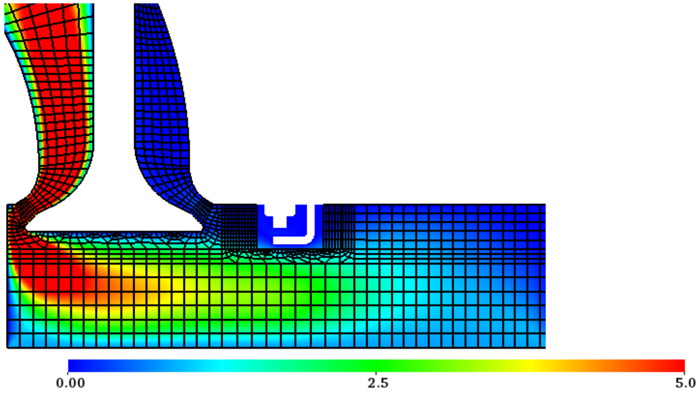
- Conduct statistical analysis to characterize turbulence. Utilize Nek5000 in "post-production" mode to gather ensemble-averages (mean and rms) of the flow-field and relevant species scalars. Generate ensemble-averaged field files for visualization purposes to qualitatively compare with experimental results. Data is immediately **archived** for future use.

NEKNEKNEK OVERSET MESHING STRATEGY

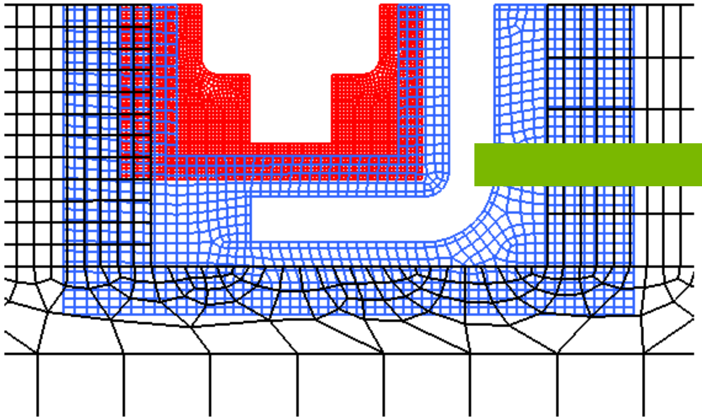
Mesh motion of outer domain

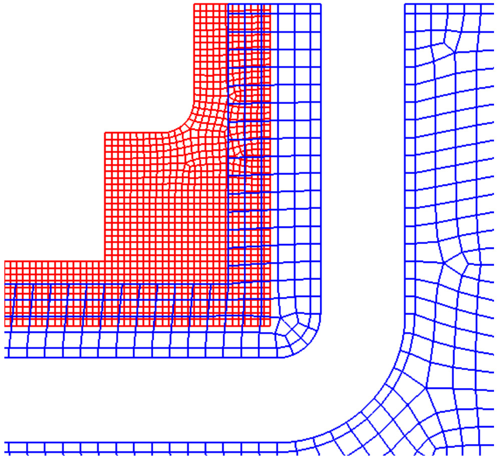


Velocity Magnitude of three domains



Interfaces/overlap between the three domains

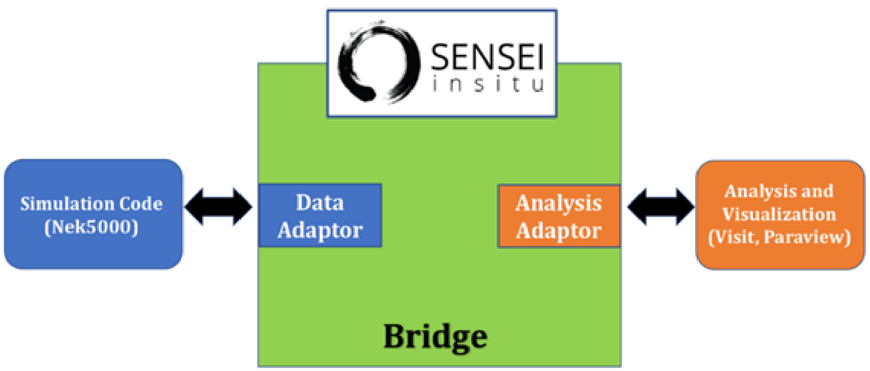




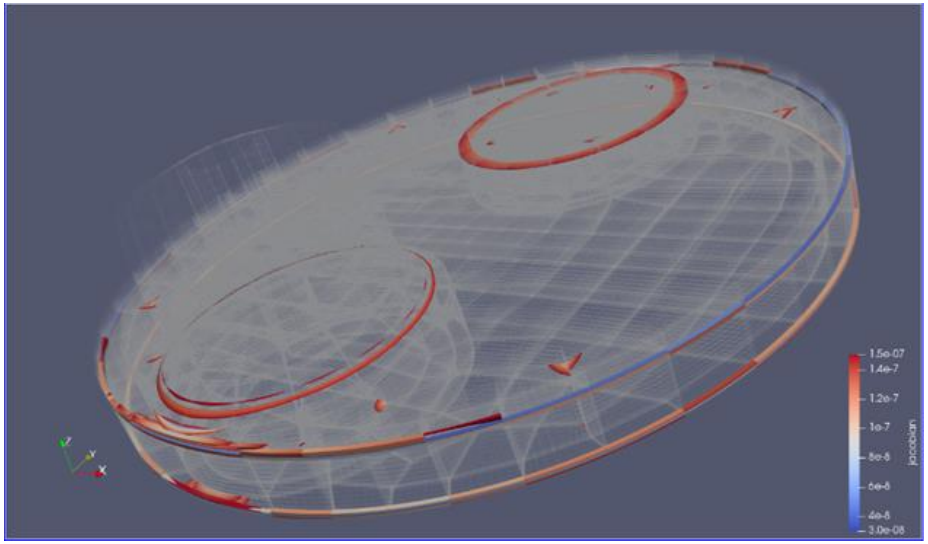
Interfaces/overlap between the inner domain containing electrode and ground strap

IN-SITU ANALYSIS WITH SENSEI

- High-fidelity ICE simulations generate 100s of TBs of data
- In-situ analysis can enhance ICE simulations by delivering inter-CAD visualization and analysis
- NEK5000 was instrumented with SENSEI in-situ framework
- As a proof-of-concept, this framework was used to better understand the mesh quality during piston and valve motion
- This will be used for future engine simulations



Schematic of how Nek5000 is instrumented with SENSEI



SENSEI interface showing the badly deformed meshes (red) during the simulation

Collaboration with visualization team at Argonne (Joe Insley, Silvio Rizzi)

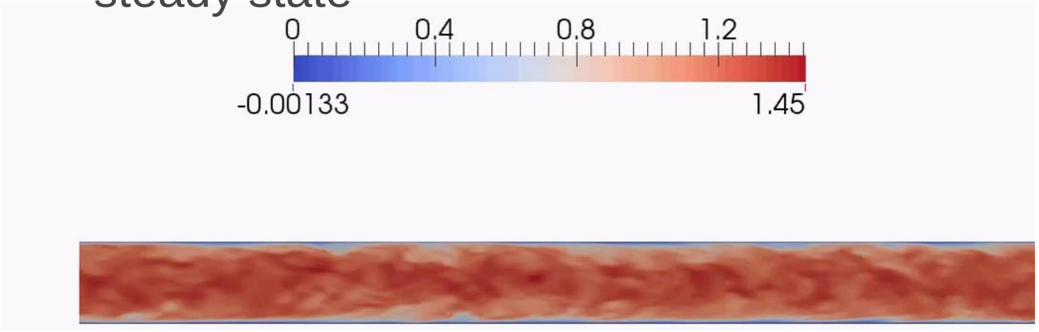
TURBULENT PIPE FLOW SIMULATIONS

Objective: Towards simulating fuel-air mixing and combustion using Nek5000

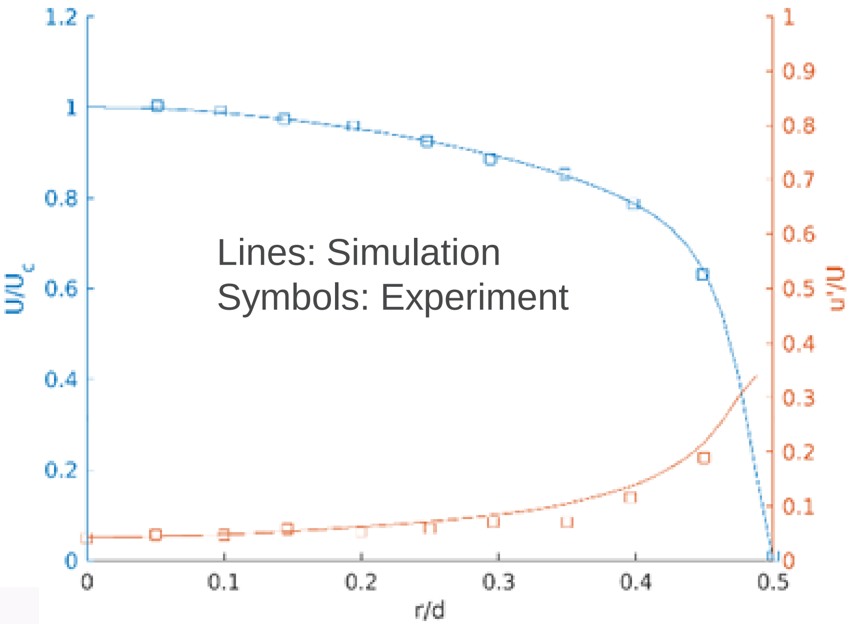
- Perform LES of non-reacting turbulent round jet
- Compare simulation results with experimental data from Vouros and Panidis (2004) with Re=5500

Approach:

- Use exact geometric details and boundary conditions
- Perform a standalone turbulent pipe flow simulation to generate accurate turbulent inflow boundary conditions for the jet simulation
- Simulations performed in a pipe of length 100D with recycling boundary condition
- Simulations continued till statistical steady state



Video showing the non-dimensional axial velocity in the pipe



Mean and RMS velocity distributions at the pipe flow exit compared to experimental measurements